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Fast delocalization leads to robust long-range excitonic transfer in a large quantum chlorosome model

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Abstract

© 2015 American Chemical Society. Chlorosomes are efficient light-harvesting antennas containing up to hundreds of thousands of bacteriochlorophyll molecules. With massively parallel computer hardware, we use a nonperturbative stochastic Schrödinger equation, while including an atomistically derived spectral density, to study excitonic energy transfer in a realistically sized chlorosome model. We find that fast short-range delocalization leads to robust long-range transfer due to the antennae's concentric-roll structure. Additionally, we discover anomalous behavior arising from different initial conditions, and outline general considerations for simulating excitonic systems on the nanometer to micrometer scale.

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Keywords

Chlorosome, exciton, graphics processing unit, green sulfur bacteria, photosynthesis, spectral density